IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oClOx41

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$HO + CHFCl_2$ (HCFC-21) $\rightarrow H_2O + CFCl_2$

$\Delta H° = -83.2$ kJ mol^{-1}

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$(2.6 \pm 0.4) \times 10^{-14}$	296 ± 2	Howard and Evenson, 1976	DF-LMR
$1.75 \times 10^{-12} \exp[-(1253 \pm 151)/T]$	298-422	Perry et al., 1976	FP-RF
$(2.7 \pm 0.3) \times 10^{-14}$	298.4		
$1.87 \times 10^{-12} \exp[-(1245 \pm 26)/T]$	245-375	Watson et al., 1977	FP-RF
$(2.88 \pm 0.24) \times 10^{-14}$	298		
$1.16 \times 10^{-12} \exp[-(1073 \pm 40)/T]$	241-396	Chang and Kaufman, 1977	DF-RF
$(3.04 \pm 0.11) \times 10^{-14}$	296		
$4.8 \times 10^{-12} \exp[-(1400 \pm 100)/T]$	293-413	Clyne and Holt, 1979	DF-RF
$(3.54 \pm 0.26) \times 10^{-14}$	293		
$(3.39 \pm 0.87) \times 10^{-14}$	297	Paraskevopoulos et al., 1981	FP-RA
$1.97 \times 10^{-18} T^{1.94} \exp[-(382 \pm 413)/T]$	250-483	Jeong and Kaufman, 1982;	DF-RF
$(3.37 \pm 0.22) \times 10^{-14}$	295	Jeong et al., 1984	
$1.53 \times 10^{-15} T^{1.11} \exp[-(1078 \pm 262)/T]$	295-810	Fang et al., 1996	PLP-LIF
$(2.48 \pm 0.67) \times 10^{-14}$	295		

Preferred Values

Parameter	Value	*T*/K
k /cm^3 molecule^{-1} s^{-1}	2.9×10^{-14}	298
k /cm^3 molecule^{-1} s^{-1}	$1.04 \times 10^{-12} \exp(-1065/T)$	240-300
Reliability		
$\Delta \log k$	± 0.08	298
$\Delta(E/R)$	± 150	240-300

Comments on Preferred Values

The absolute rate coefficients of Clyne and Holt (1979) are significantly higher than those of Howard and Evenson (1976), Perry et al. (1976), Watson et al. (1977), Chang and Kaufman

(1977), Paraskevopoulos et al. (1981), Jeong and Kaufman (1982) and Fang et al. (1996), and are therefore not used in the evaluation. The absolute rate coefficients of Howard and Evenson (1976), Perry et al. (1976), Watson et al. (1977), Chang and Kaufman (1977), Paraskevopoulos et al. (1981), Jeong and Kaufman (1982) and Fang et al. (1996) have been fitted to the three parameter equation $k = CT^2 \exp(-D/T)$, resulting in $k = 2.00 \times 10^{-18} T^2 \exp(-535/T)$ cm^3 molecule^{-1} s^{-1} over the temperature range 241-810 K. The preferred Arrhenius expression, $k = A \exp(-B/T)$, is centered at 265 K and is obtained from the three parameter equation with $A = C e^2 T^2$ and $B = D + 2T$.

References

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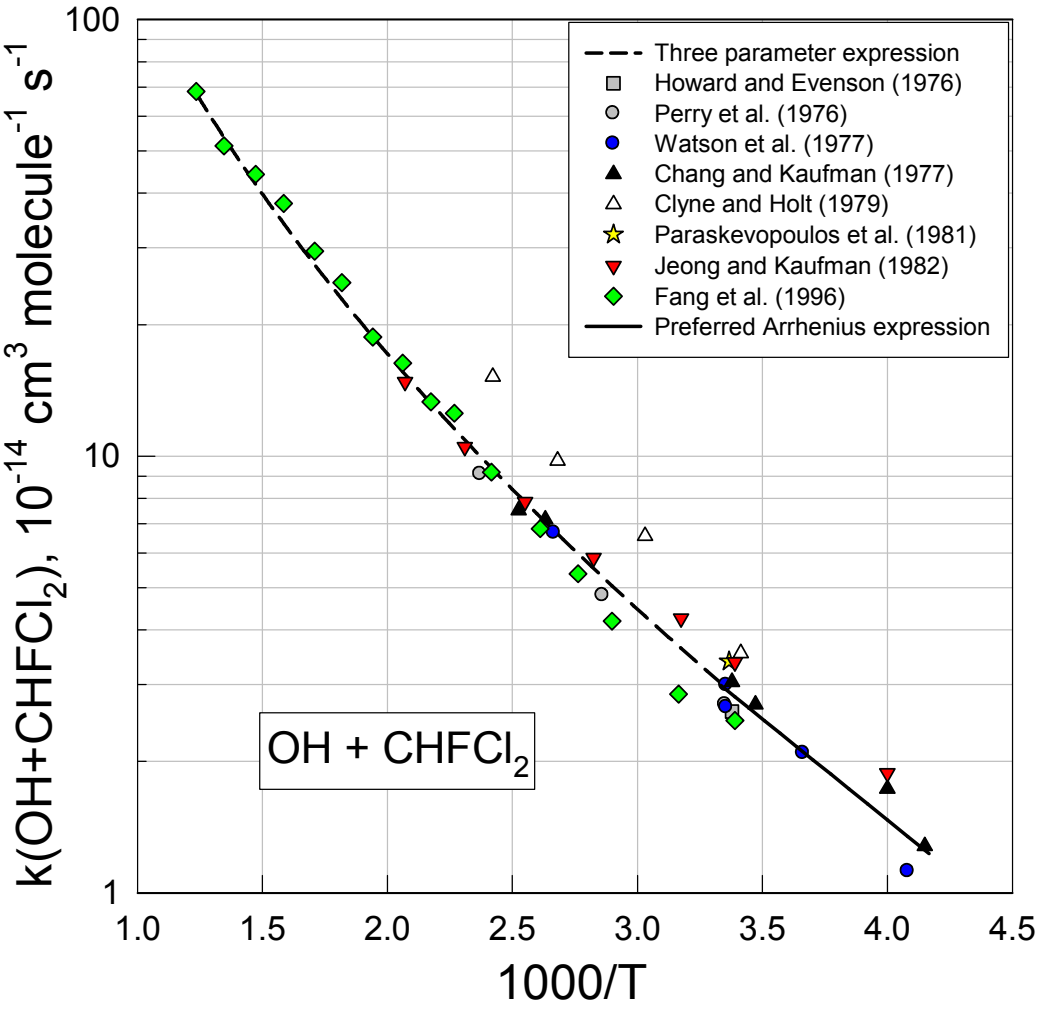
Three parameter expression
Howard and Evenson (1976)
Perry et al. (1976)
Watson et al. (1977)
Chang and Kaufman (1977)
Clyne and Holt (1979)
Paraskevopoulos et al. (1981)
Jeong and Kaufman (1982)
Fang et al. (1996)
Preferred Arrhenius expression
OH + CHFCl2
k(OH+CHFCl2), 10-14 cm3 molecule-1 s-1
1000/T
100
10
1
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5